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Professor Dow

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Arixona Board of Regents, Acting for and on Behalf of Arizona State University
Box 871603
Tempe AZ 85287-1603

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13. ABSTRACT (A

This report summarizes work performed on novel semiconductor materials. A new sp^3d^5 empirical tight-binding model of the electronic structure of silicon was developed. Models showed that the Er^{+3} crystal-field splitting in Si has a different electronic structure than previously assumed in the literature. Surface reconstructions of Si have been worked out for 5-by-1 and 16-by-2, the latter of which is the largest ever described. A theory describing the role of interfacial charges in determining lattice-matching conditions at substrate surfaces was developed. The defect structure of the first successful STM image of the GaN(0001) surface on a mismatched substrate was modeled. Electronic structure calculations showed that quantum dots, which can result from controlled lattice-mismatched growth, have indirect bandstructure under certain conditions. Finally, the conventional theory of superconductivity is called into question with the determination that the primary superconducting condensate resides in the charge resevoir layers, as opposed to occupying the cuprate planes.

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Arizona State University

John D. Dow, Professor
Department of Physics and Astronomy
Arizona State University, Station 871504
Tempe, Arizona 85287-1504 U.S.A.
Office phone: (602) 965-1949
Departmental secretary: (602) 965-3561
Home phone: (602) 423-8540
FAX: (602) 423-5183
Email (last resort): dow@dowjd.la.asu.edu

9 October 1997

Maj. Michael Prairie
Air Force Office of Scientific
Research (AFMC) - NE Building 410
110 Duncan Avenue, Suite B115
Bolling AFB, DC 20332-0001

RE: Final report

Dear Major Prairie,

This is a summary of work completed under contract/grant AFOSR-F49620-94-10163 in its final year.

Semiconductors

We have developed a new sp^3d^5 empirical tight-binding model of the electronic structure of Si, which should prove useful for modeling the valence bands and lowest conduction bands of Si.

We have performed the first successful imaging of the GaN(0001) surface by scanning tunneling microscopy and presented models of the defect structures observed.

We have developed a theory of substrates and the role of interfacial-charge in determining a correction to the lattice-match condition.

We have worked out the physics of crystal-field splitting of Er^{+3} in Si, finding a different electronic structure from the structure that has been assumed.

We have constructed models of the "16×2" and "5×1" surface reconstructions of Si(110). The "16×2" reconstruction has one of the largest surface unit cells ever worked out.

We have shown that quantum dots are likely to exhibit unanticipated phenomena, including (i) valence band maxima that were at **k=0** in the bulk which are displaced from **k=0** by an amount of order D^{-1} in the dot, where D is the dot diameter (direct bulk semiconductors become indirect in quantum dots), and (ii) dopants that are deep traps in the dots, which were shallow impurities in the bulk.

Superconductors

We have shown that the charge-transfer hypothesis, which lies at the foundation of most theories of high-temperature superconductivity, is contradicted by the very data once thought to support it.

We have shown that the effects of Ni and Zn doping of high-temperature superconductors are the same in all materials measured to date, except $Nd_{2-z}Ce_zCuO_4$, which exhibits BCS-like behavior. This contradicts most of the popular theories, but is fully consistent with our charge-reservoir-oxygen model of superconductivity.

We have developed an understanding of $Sm_{1.5}Ce_{0.5}Sr_2Cu_2NbO_{10}$ and its superconductivity, predicting its critical temperature, and predicting the effects of Ni and Zn doping.

We have demonstrated that the spin-fluctuation d-wave pairing model of high-temperature superconductivity is contradicted by its own self-test, hopefully eliminating this popular model from further consideration.

We have shown how pair-breaking can be employed to locate the primary superconducting condensate — which invariably occupies the charge-reservoir layers of high-temperature superconductors, not the cuprate-planes.

We have proposed that *all* high-temperature superconductors are *p*-type, and have proposed a model of *p*-type doping in $Nd_{2-z}Ce_zCuO_4$ (which has been assumed to be *n*-type) in terms of (Ce,interstitial oxygen) pairs.

As I look at the three-year proposal and the annual reports, I believe that the proposed work has been done, and other, unanticipated work has led to very interesting breakthroughs.

I hope that you feel you have gotten your money's worth.

It has been a pleasure working for you. If I can be of help in the future, do not hesitate to call on me.

Thank you very much for your support.

Sincerely,

John D. Dow
Professor

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Principal Investigator Annual Data Collection Form (PIADC)

PI Name (Last, First, MI): Dow, John D.

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Institution: Arizona State University
Department of Physics and Astronomy
Tempe, AZ 85287-1504
Contract/Grant No.: AFOSR-F49620-94-10163

A. Publication in Reviewed Journals

Ren, Shang-Yuan, Xia Chen, and Dow, John D., Tight-binding sp^3d^5 Hamiltonian for Si. J. Phys. Chem. Solids, in press.

Blackstead, Howard A. and Dow, John D., Charge-transfer in $YBa_2Cu_3O_x$. J. Superconduct. **9**, 563-578 (1996).

Blackstead, Howard A. and Dow, John D., Ni and Zn doping of Cu sites in superconducting $Nd_{2-z}Ce_zCuO_4$, $La_{2-\beta}Sr_\beta CuO_4$, $Bi_2Sr_2CaCu_2O_8$, $Bi_{1.8}Pb_{0.2}Sr_2Ca_2Cu_3O_{10}$, $YBa_2Cu_3O_7$, $La_{0.6}Ca_{0.4}Ba_{1.35}La_{0.65}Cu_3O_x$, and $YBa_2Cu_4O_8$. Philos. Mag. **B 74**, 681-714 (1996).

Blackstead, Howard A., Dow, John D., and Pulling, David B., Theory of $Sm_{1.5}Ce_{0.5}Sr_2Cu_2NbO_{10}$: Critical-Temperature and Doping Effects. J. Low Temp. Phys. **105**, 705-710 (1996).

Blackstead, Howard A. and Dow, John D., Absence of magnetic pair-breaking by Ni in most high-temperature superconductors. J. Low Temp. Phys. **105**, 699-704 (1996).

Packard, William E., Dow, John D., Doverspike, Kathleen, Kaplan, Ray, and Nicolaides, Ruth, Vacancy structures on the GaN(0001) surface. J. Mater. Res. **12**, 646-650 (1997).

Ren, Shang-Yuan and Dow, John D., Role of interfacial-charge in the growth of GaN on α-SiC and sapphire. J. Electron. Mater. **26**, 341-346 (1997).

Ren, Shang-Yuan and Dow, John D., Crystal-field splitting of Er^{+3} in Si. J. Appl. Phys. **81**, 1877-1882 (1997).

Blackstead, Howard A. and Dow, John D., Occurrence of spin-fluctuation pairing in high-

temperature superconductors. Submitted.

Packard, William E. and Dow, John D., Si(110)–"16×2" and Si(110)–"5×1" surface reconstructions: Stretched-hexagon, face-centered adatom model. Phys. Rev. **B 55**, 15642-15651 (1997).

Blackstead, Howard A. and Dow, John D., Absence of exchange scattering by cuprate-plane impurities in high-temperature superconductors. *Proc. 10th Anniversary HTS Workshop on Physics, Materials, and Applications,* edited by B. Batlogg, C. W. Chu, W. K. Chu, D. U. Gubser, and K. A. Müller (World Scientific, Singapore, 1996), pp. 485-486.

Blackstead, Howard A. and Dow, John D., Evidence that all high-temperature superconductors are *p*-type. Phys. Rev. **B 55**, 6605-6611 (1997).

B. Books or Book Chapters Published

None.

C. Graduate Students

None.

D. Post-Doctorates

Ren, Shang-Yuan, Physics and Astronomy, non-US
Packard, William E., Physics and Astronomy, US

E. Awards, this year

Dow, John, D., Certificate of Appreciation, Battelle, 1997

E'. Awards, this year, Ren, S.-Y.

Distinguished University Professorship, Peking University, 1994-present

E". Awards, previous years, Dow, J. D.

Dow, John, D., National Defense Science and Engineering Appreciation Award, Oak Leaf Cluster, 1994, 1995, and 1996
Dow, John, D., Certificate of Appreciation, Battelle, 1994, 1995, and 1996
DuPont Educational Aid Award 1993 (unsolicited) ($10,000)
Battelle National Defense Science and Engineering Appreciation Award, 1993
DuPont Educational Aid Award 1992 (unsolicited) ($8,000)
Distinguished University Professor, Arizona State University, Spring, 1990

Frank M. Freimann Professor of Physics, University of Notre Dame, 1983-1991
Permanent Honored Guest Professor, Tsinghua University, Beijing (The other two recipients of this award are Nobel Laureates T. D. Lee and C. N. Yang), 1989-present
Elected an alumnus member of Phi Beta Kappa, 1989
Award for contributions to North Dakota's efforts at enhancing science excellence, 1988
Awarded a 1987 Mercury Sable X-Plan Automobile in recognition of contributions to theoretical physics, by the Ford Motor Company
Certificate of citation from the State of Indiana, Office of Governor Robert D. Orr, for outstanding leadership in Science and Technology, 1987
Certificate of Recognition of the Materials Research Society, 1987
Ford Motor Company Research Award ($15,000), 1983-7
Board of Directors, I/O Experts, Inc., Willoughby, Ohio, 1985-
Visiting Professor of Chemical Engineering and Materials Science, University of Minnesota, 1987
Visiting Professor of Physics, University of Science and Technology of China, Hefei, 1986
Visiting Scientist, Scuola Normale Superiore, Pisa, Italy, 1981
Unidel Visiting Professorship, University of Delaware, 1978
Associate, Illinois Center for Advanced Study, 1976-7
Fellow, American Physical Society, 1976
National Science Foundation Postdoctoral Fellow (Princeton University), 1967-8
NASA fellow (University of Rochester), 1966-7
Who's Who in Technology Today
American Men and Women of Science
Who's Who in Engineering
Men of Achievement, International Biographical Centre, Cambridge